Overview of SBC robotic sample changer operations:

The SBC bending magnet automated sample mounting system increases crystallographic data collection throughput and decreases the amount of work required by the user. Currently, available functionality includes automated crystal mounting, crystal exchanging and crystal dismounting, click-to-center crystal alignment, and phosphor mounting. These features make the automated system quicker than manual operations.

This document outlines the loading of samples into magazines, the loading of the magazines into the robot dewar, the starting of the robot, and the shutdown of the robot. In addition there are two appendices: Appendix A: *Magazine location diagram* and Appendix B: *Error codes and recovery procedures*. The information required to perform standard sample mounting operations is contained in these sections.

Loading of samples into magazines:

These sample handling operations should be finished before the scheduled beamtime. **Practice** inserting empty sample holders into the magazines (pucks) **before performing this task with mounted crystals**. The samples are placed in the magazines **upside down**, seated on the magnetic posts at the bottom of the holes.

There is a sticker on each magazine, designating the numbering scheme for the sample wells. Write down the location and magazine color for each sample so the crystal can be tracked throughout the data collection process. The location of each crystal can be entered into a comma separated value file (CSV) that can be downloaded from the SBC website.

Hampton Research has recently introduced a new style of sample holders

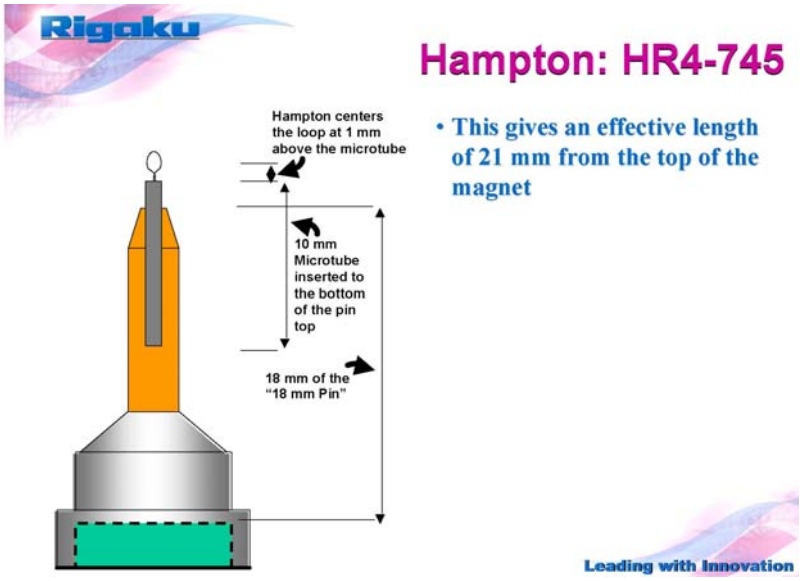


Figure 1. Robot compatible pin dimensions.

Step by step: Loading the magazines

1. Obtain robot compatible sample holders—*18mm pins* (21mm from magnet to loop) *and verified base diameter,* see Figure 1. The base diameter should be checked with the magnetic wand, use the **red** end.
2. Mount and freeze the crystals on the previously checked sample holders. It is convenient to temporarily store the samples right side up in one of the small wire racks.
3. Place an empty magazine in the large diameter, short dewar equipped with the metal plate. This dewar will hold the magazines at a convenient height for insertion of the sample holders.
4. Use the magnetic wand to transfer the frozen samples, one at a time, to the dewar with the magazine.
5. Use a pair of cryovial tongs to turn the sample upside down.
6. Insert the samples into a magazine.
    - **Practice this operation with a room temperature puck and empty sample holders.**
    - Use the Rigaku tweezers or long tongs, Figure 2, to transfer the previously frozen samples to the robot magazines by grasping the cryovial and dropping the cap and vial into a well in the puck. The rear of the tweezers, or another tool, can be used to wiggle the cryovial until the sample holder appears seated in the hole.

Figure 2. Rigaku tweezers.

7. Remove the cryovials by grasping them with the Rigaku tweezers. Alternatively, the magnetic wand can be used to remove the cryovials if **CrystalCap HT** sample holders are used.
8. Check each magazine position for proper sample seating, first visually, then with the sample check tool, as shown in Figure 3. First, try this operation with an empty, room temperature magazine to become familiar with the tool. The sample check tool should be inserted into **each** hole in **every** puck. The tool will slide all the way to the puck top surface if the sample is correctly positioned. Samples that are slightly off center will "click" into place during this process. If the sample doesn't click into place, put the cryovial back on the sample then try to maneuver the sample into place. Incorrectly seated samples may cause the robot to stop and cause delays during crystal mounting.
    - NOTE: A few sample have become stuck in the sample check tool. Check that this has not occurred before inserting the tool into the next hole. This does not happen frequently.

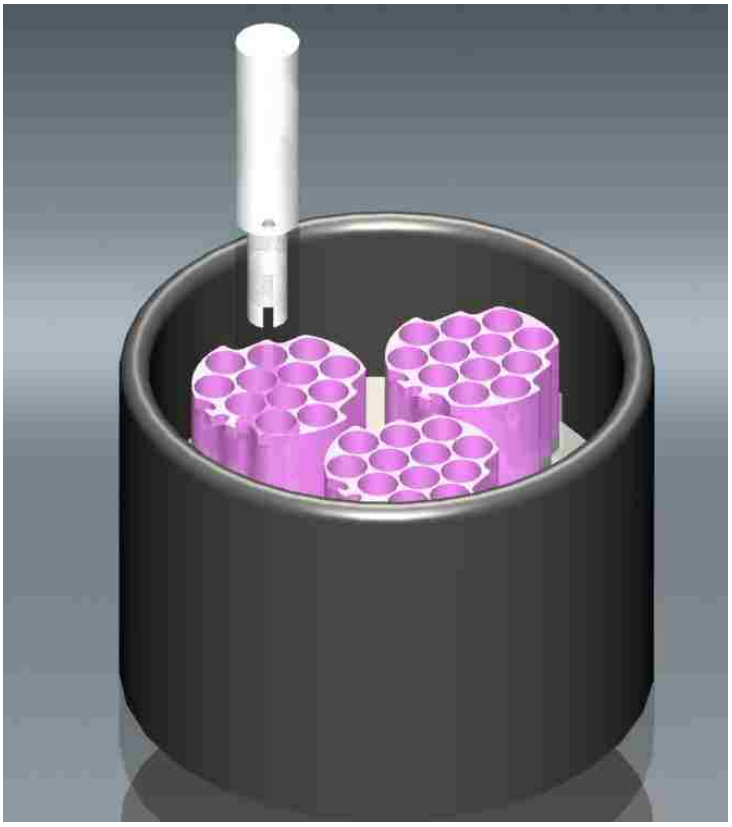


Figure 3. Usage of sample checking tool.

9. The wide dewar can be used to carry the magazines to the robot storage dewar.
10. If the samples are to be stored, place each magazine in the storage rack and then place the storage rack into a dry shipper or a storage dewar.

Placing magazines into the storage dewar and interlocking hutch:

The magazines must be inserted into the robot storage dewar before starting the robot and closing the hutch door. If possible, the magazine loading procedure should be **practiced with empty magazines at room temperature**. Magnets hold the magazines to the plate in the storage dewar. The position of each magazine is located by two pins, with two additional pins to guide the magazine during insertion. A close up of the pins on the dewar plate and the bottom of a magazine are shown in Figure 4.

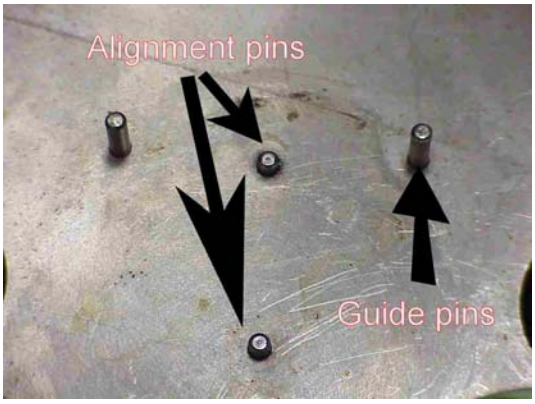


Figure 4. Dewar plate pins and magazine bottom.

Long tongs are used to place the magazines into the dewar. Once the magazine is felt to have "clicked" into place, try to rotate the magazine in the plane of the dewar bottom. A magazine that is seated correctly will not turn. Figure 5 shows the storage dewar with eight magazines inserted.

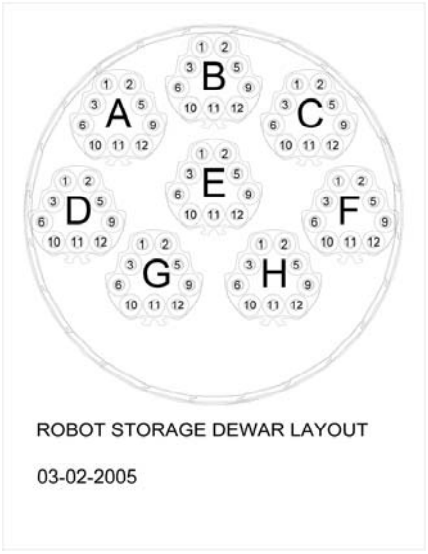


Figure 5. Storage dewar with eight magazines (left) and labeling convention (right).

The florescence detector should be positioned before searching and interlocking the hutch. The beamline control system doesn't know the location of the florescence detector tripod, so it is imperative that it is located correctly to avoid a collision with the robot. Place the tripod feet within the yellow tape boxes on the floor, shown in Figure 7. The detector can then be aligned to the sample position. If there are any questions regarding proper florescence detector placement, please ask the host for assistance. Check to see that the path between the light curtain transmitter and receiver, shown in Figure 6, is clear, then search the hutch.

Figure 6. Light curtain path.

Figure 7. Fluorescence detector position.

Step by step: Loading the storage dewar

1. Look into robot storage dewar to decide which magazine positions are available, as shown in Figure 5.
1. Dress in proper PPE before attempting to load the magazines.
2. Remove the magazine storage rack from the dry shipper or transport dewar.
3. Remove the storage rack locking bar, used to prevent shifting of the magazines.
4. Use the long tongs to engage the desired magazine at the “ears”. Close the tongs, the locking action will keep them shut. **If the magazine is to be placed in position G, the tongs will have to be rotated 180°**, with the finger holes over the magazine.
5. Slide the magazine out of the rack and place it under the liquid nitrogen within the storage dewar and wait for any boiling to cease.
6. The magazine can now be maneuvered into place. Keep the front of the magazine lower than the rear; this will aid in locating the guide pins. When the magazine has been pushed against the guide pins, allow the magnet to pull it down to the dewar base.
7. Try and gently rotate the magazine in the plane of the dewar plate; it should not move.
8. Repeat the operation for up to eight magazines, taking note in which positions, A-H, each of the magazines are placed.
9. If there are any difficulties or questions regarding the proper positioning of the magazines ask Curt Preissner (2-3020) for assistance.
10. Remove the tongs.
11. Check to see if there is a sample on the goniostat. If a sample is present, remove it.
12. Position the florescence detector tripod feet within the yellow squares on the floor.
13. Search and interlock the hutch.

System startup procedure:

The system is started from outside the hutch, after the door is closed. All of the robot operations are controlled from the *mounting* tab in *SBC Collect*, so *SBC Collect* should be started. Screen shots of *SBC Collect* are shown for reference in Figure 11 through Figure 13.

The buttons and message areas concerning the robot are grouped in one section of the *mounting* tab; see Figure 10. The *Robot Online* light indicates whether or not the robot is ready to perform crystal operations; green indicates the robot is running and red that it is stopped. The robot is started using the *Start* button and stopped using the *Shutdow*n button; however, the robot is interlocked to the hutch door. Anytime the hutch door is opened, **including when a sample is in transit**, the robot will enter the shutdown state and will need to be restarted upon closing the hutch door. The *Start* operation moves the robot from the *storage* position, Figure 8, to the *park* position, Figure 9. In order to prevent the loss of a sample, the user should shut the robot down before entering the hutch. Press the *SHUTDOWN* button, and then make certain, by checking the *Robot status* message and *Robot Online* light, that the robot has completed the shutdown operation. When the robot is offline, the hutch door can be opened.

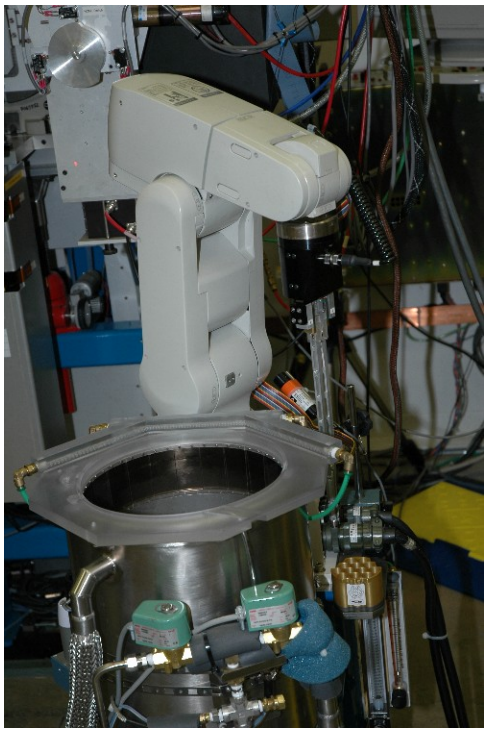


Figure 8. Robot storage position.

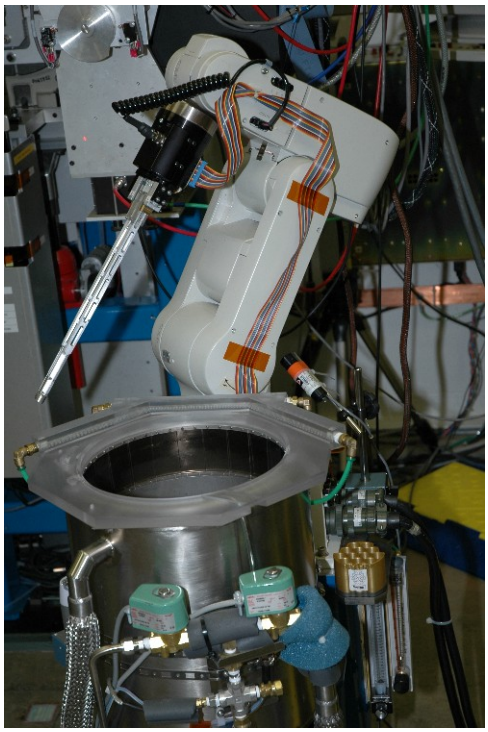


Figure 9. Robot park position.

Important information about the system is relayed to the user through the *Beamline status*, *Robot status*, and *Error #* message areas. In addition, the *Mounted sample* window contains the number of the currently mounted sample or tool. If this area is blank, the goniometer is empty. There are specific buttons for *Mounting*, *Exchanging*, and *Dismounting* samples, along with a button to mount a phosphor. The meaning of error messages displayed in the *beamline status* window can be indexed in Appendix B.

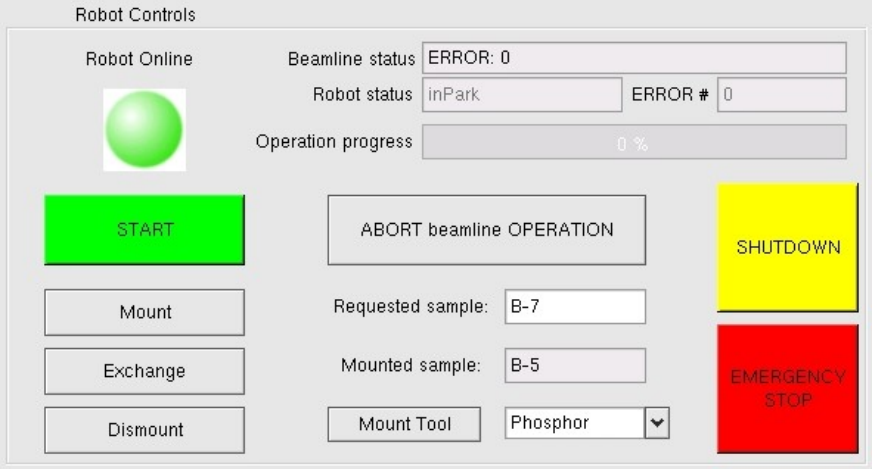


Figure 10. SBC Collect robot controls.

Step by step: Starting the robot

1. Run *SBC Collect* from the red toolbar (SBCTOOLS) or from a terminal window.
2. Click on the *mounting* tab, shown in Figure 12, to access the robot controls.
3. Click on the *Data Source/File* button to load your previously defined CSV sample file, or choose the default sample information template: *robot-template.sample*.
4. Click the green *START* button.
5. Wait for the *Robot started OK!* message to be displayed in the *Beamline status* area and wait for the *Robot Online* light to turn green. It will take a short amount of time for the robot to move into position and come online.

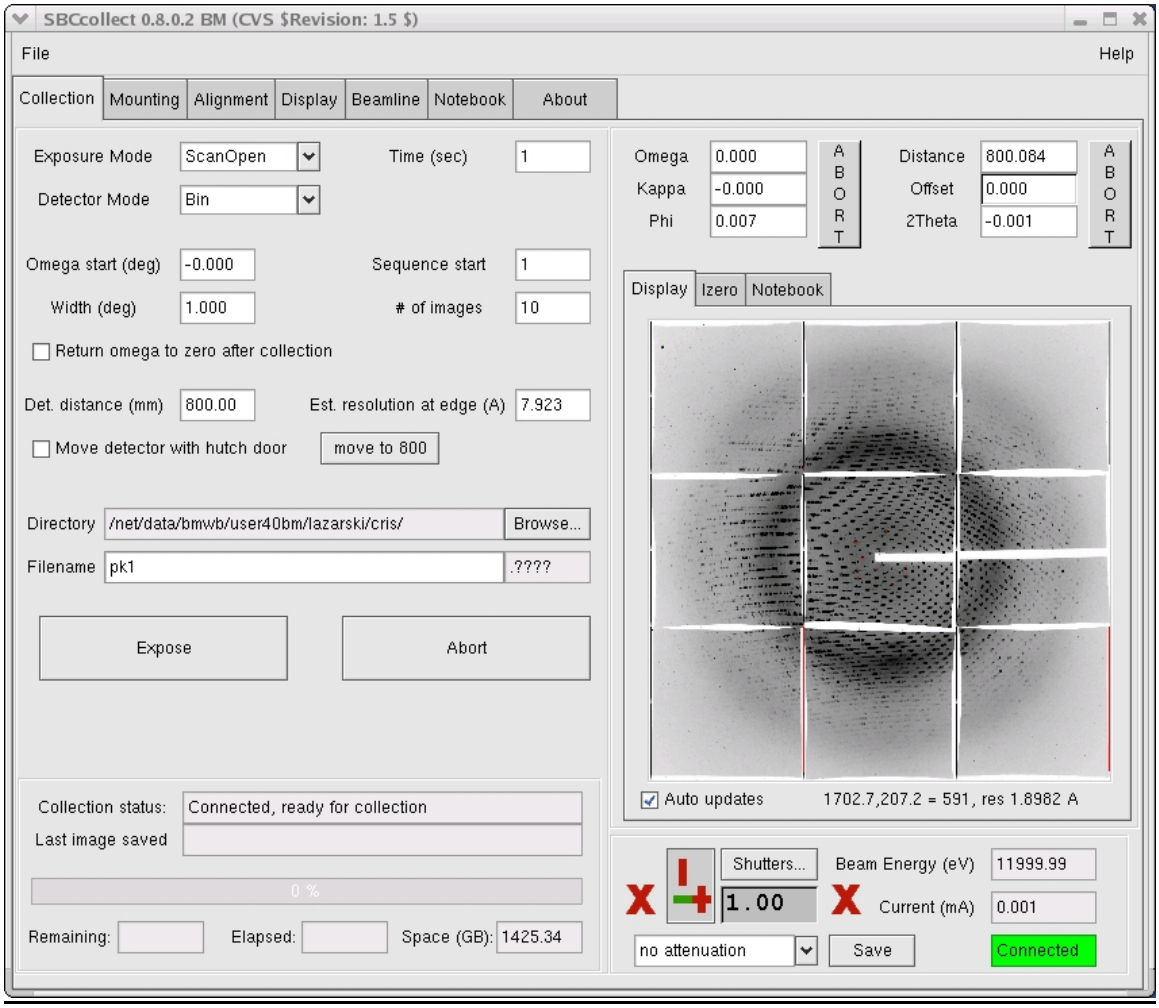


Figure 11. SBC Collect, data collection tab.

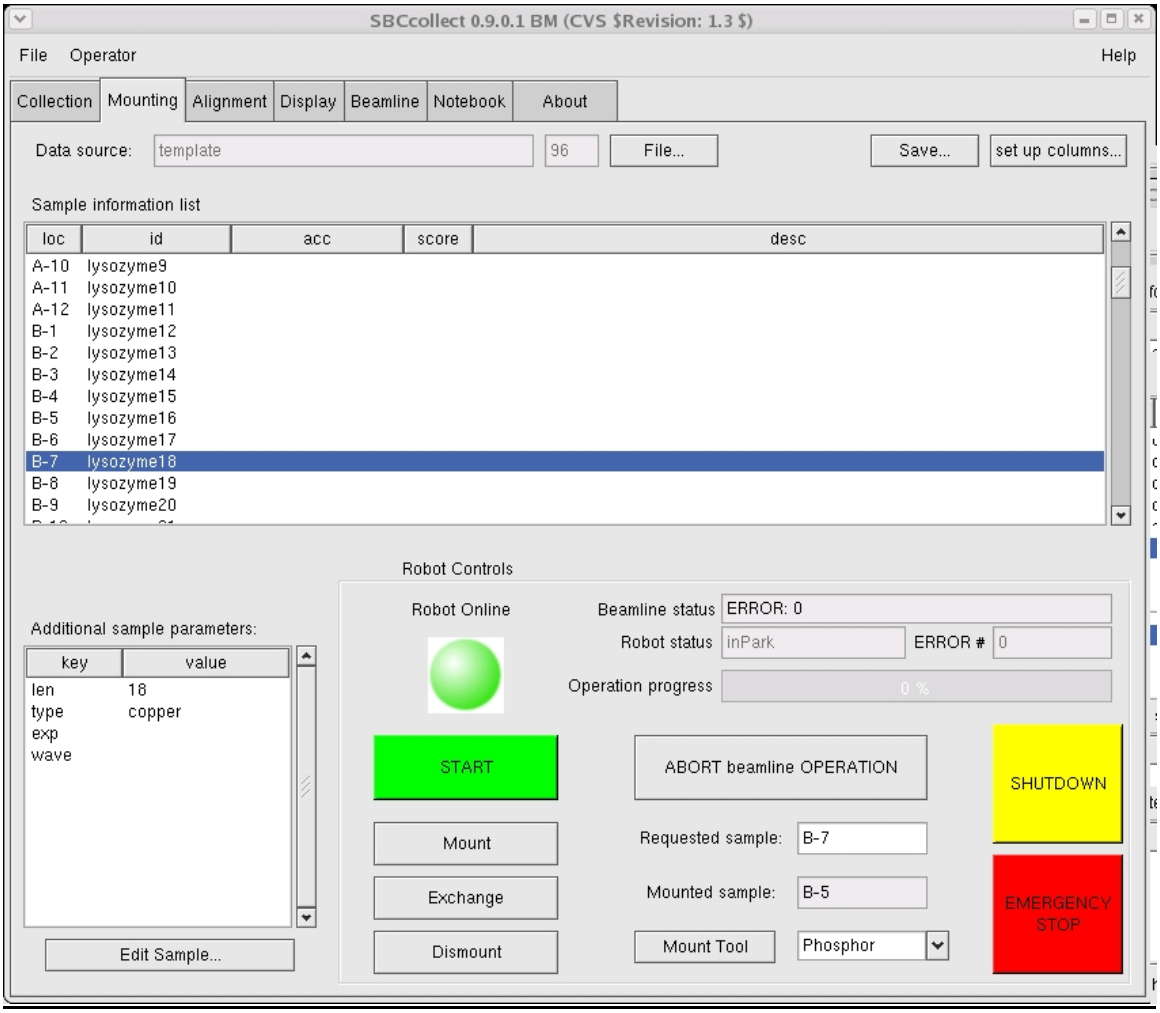


Figure 12 SBC Collect, mounting tab.

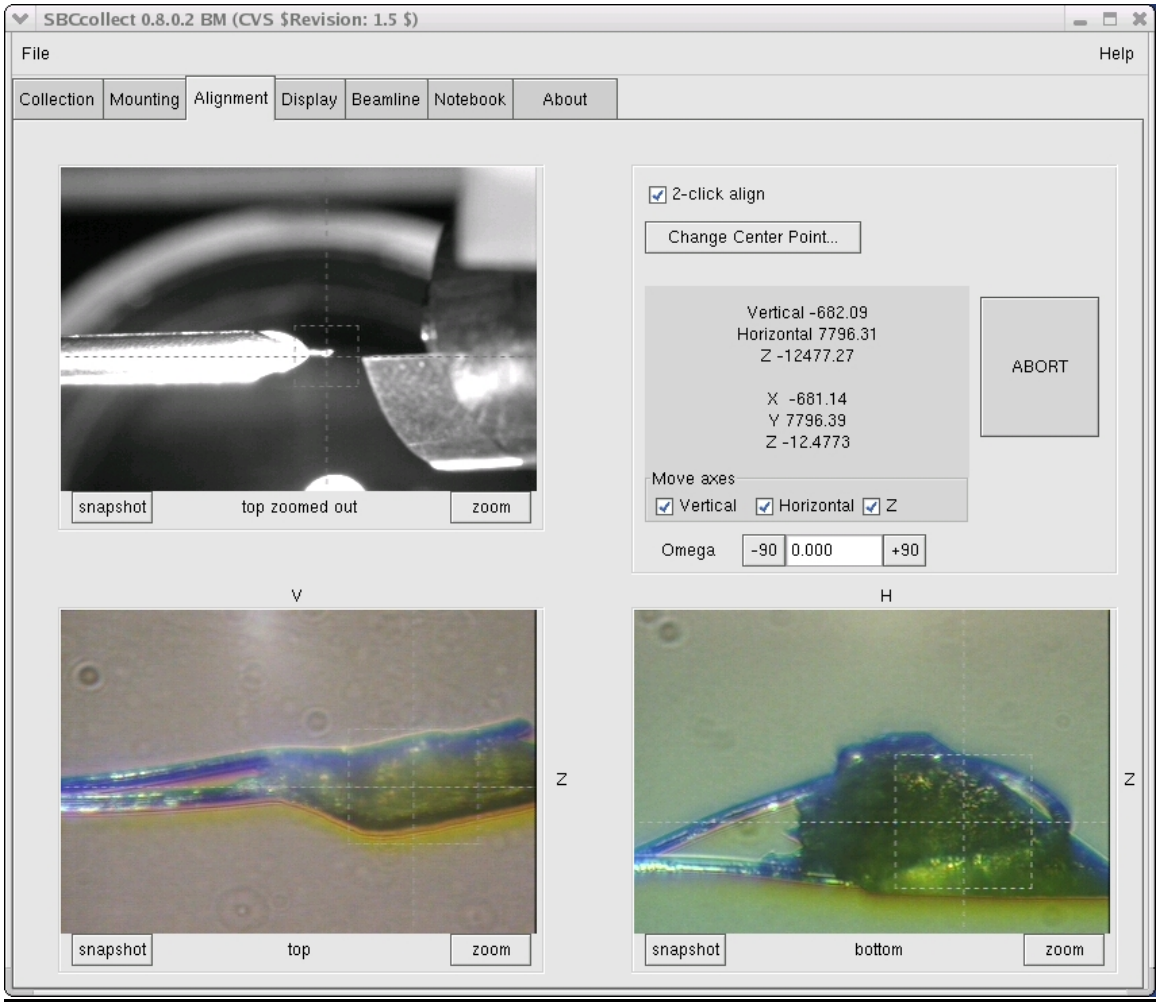


Figure 13. SBC Collect, alignment tab.

Using the robot during data collection:

A brief description of typical data collection operations is detailed below. The operations are again outlined in a workflow chart. Explicit instructions for carrying out data collection are outlined in the *Step by step* section.

Once the hutch is interlocked and the robot is running, data collection operations can begin. As with manual operations, the first task is to locate the beam and align the goniometer omega axis to the beam position. The phosphor is selected from the *Tool selection* dropdown menu and is mounted by clicking the *Mount Tool* button. The robot system will automatically move the goiniostat to the position and orientation at which the robot gripper can interface with the goniometer, mount the phosphor, and then return the goniostat to a location close to the beam location. *Tool mounted* will be displayed in the beamline status window when the operation is complete. The phosphor can then be oriented normal to the beam and moved into position by using the functionality available through the *Alignment* and *Collection* tabs in *SBC Collect*. After the beam position has been verified, the location of the goniostat should be saved by clicking the *Learn Rotation Axis* button under the *Beamline* tab. The phosphor is removed by clicking the *Dismount* button on the *Mounting* tab.

After the beam position has been determined, the first sample will be placed on the goniostat using a *Mount* operation. The sample can subsequently be *Exchanged* with another sample, or *Dismounted*. The *Exchange* operation is used to quickly replace the mounted sample with another sample, and then proceed with data collection. The robot gripper doesn't need to be dried in between samples when the *Exchange* process is used, thus reducing cycle time. This is because the robot gripper does not leave the storage dewar between samples. The *Dismount* operation removes the mounted sample, and then dries off the gripper. The phosphor can only be mounted when there is no sample on the goniostat.

The typical workflow is shown in Figure 14. The maroon arrows follow the workflow if the robot has not been used during data collection recently. The blue arrows follow the path taken if the beamline has been set up for robot operations. Remember, shut the robot down and wait for it to go offline before entering the hutch.

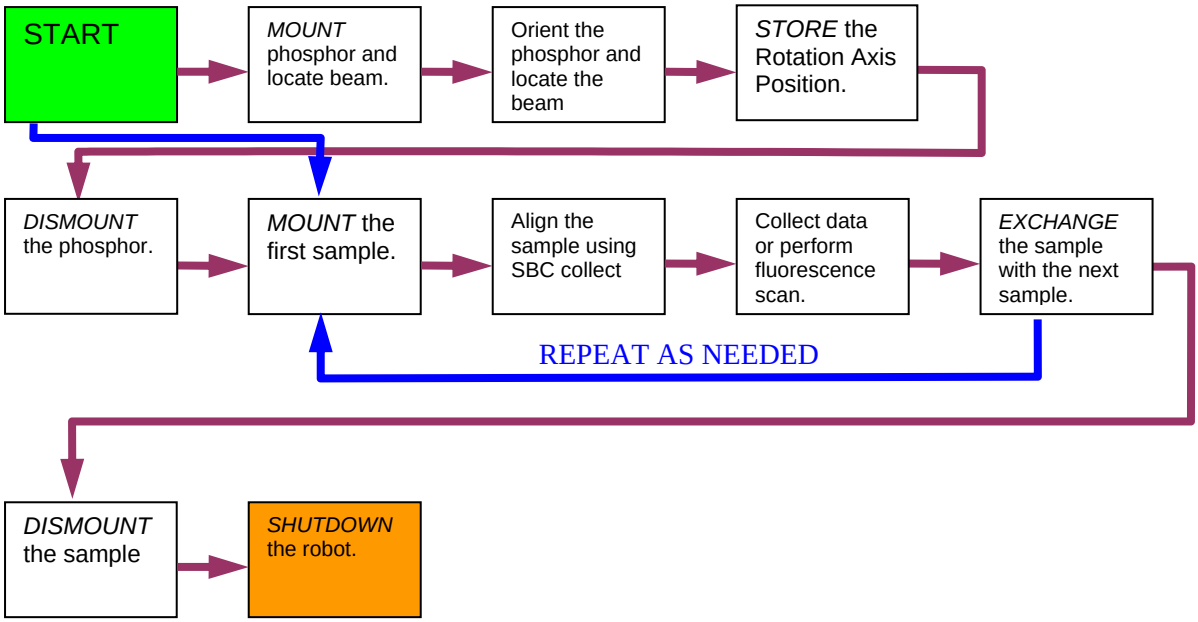


Figure 14. Workflow diagram.

Step by step: Robot use during data collection

1. Click the *Mounting* tab on *SBC Collect*, see Figure 12.
2. Check that the *Robot Online* light is green, if not press the *START* button.
3. Use the *Tool selection* dropdown menu to select the phosphor.
4. Click *Mount Tool* to initiate the phosphor placement. Watch for the *Tool mounted* message.
5. After the phosphor has been mounted, go to *Alignment* tab and use standard operating procedures to move the goniostat to the beam position, determine proper focus, etc…
6. Under the *Beamline* tab on *SBC Collect*, press the *Learn Rotation Axis Position* button. The position of the goniometer will be stored. This will become the position that the goniostat returns to after a sample is mounted or exchanged.

7. Press the *Dismount* button to remove the phosphor. The message box will display *dismount completed* when the operation is finished.
8. Enter the sample to be mounted into the *Requested sample* box, either by clicking on the desired sample in the listing window, or typing a value.
9. Press the *Mount* button. *SBC Collect* will move all of the beamline equipment into the mounting position, and then initiate the robot mount sequence. When the mounting sequence is completed, *SBC Collect* will move all of the beamline equipment back to the data collection position (the position that was stored in step 6).
10. Click the *Alignment* tab on *SBC Collect,* Figure 13.
11. First, align the sample using the wide-field camera in the upper left. Clicking on the loop will bring that position to the crosshairs.
12. Click the buttons to extend the reflector and turn the lights on as needed.
13. Use either the horizontal or vertical high magnification views to center the crystal on the crosshairs. It shouldn't take more than one click in each window to achieve a good center. If the Z position is acceptable, the Z axis can be deactivated in order to speed up the alignment.
14. Click the *Collection* tab on *SBC Collect,* Figure 11.
15. Proceed with diffraction data collection in the standard way. When finished, return to the *Mounting* tab.
16. If no other crystals are to be mounted, click the *Dismount* button. This will remove the crystal from the goniostat.
17. If data is to be collected on another crystal, enter the desired crystal number into the *Requested sample* box.
18. Press the *Exchange* button, causing the robot to remove the mounted crystal and mount the next crystal.
19. Repeat the exchange and alignment processes with other crystals. Use the *Dismount* command to remove the final crystal.
20. Press the *Shutdown* button to move the robot to the storage position.

A few reminders…

- Beamline tools can be mounted any time the goniostat is empty.
- The robot should be offline (*Robot offline* light is red) before entering the hutch. Pressing the *Shutdown* button will move the robot to the storage position and shut it down, providing the clearest path to the goniostat.
- The robot will shutdown anytime the hutch is opened, including when it has a sample in the gripper, causing loss of the sample. Verify that any robot operation has completed before entering the hutch. This can be done by looking in the message window or observing the hutch camera. The robot should be in either the *park* or *storage* position. If the robot is inadvertently stopped while drying or while cooling, close the hutch door and press the *START* button to return the robot to the park position.

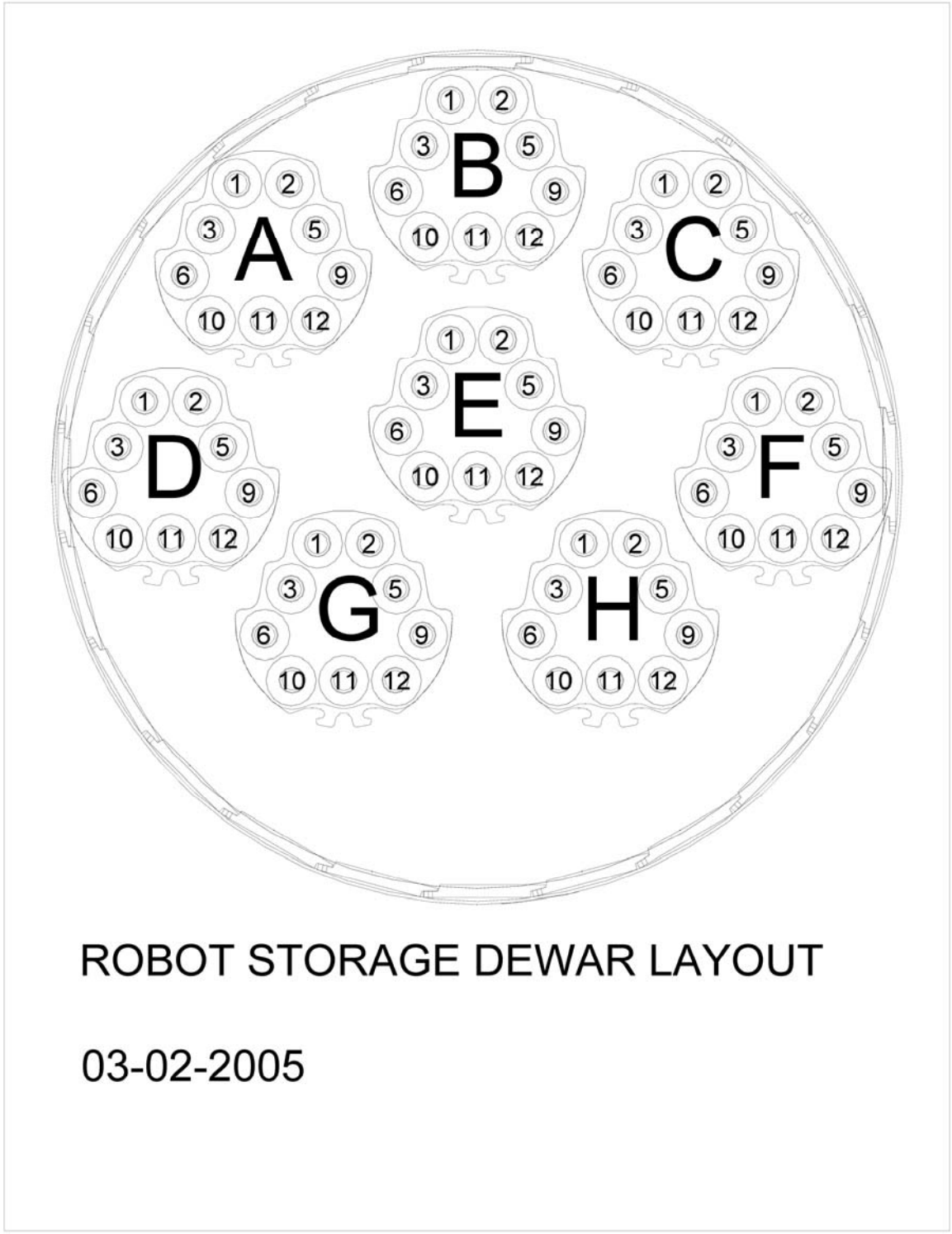
System shutdown procedure:

The robot should be placed in a shutdown state whenever operations are complete or the beamline is going to be left unattended for a long period of time.

Step by step: Shutting the robot down and removing magazines

1. Check to see if the robot is in the *storage* position.
2. Press the *Shutdown* button to move the robot to the storage position. If the robot is offline, it will have to be started before it can be shutdown correctly.
3. Enter the hutch when the *Robot offline* light is red.
4. Dress in proper PPE before removing the magazines from the storage dewar.
5. Fill the transfer dewar or shipping dewar with liquid nitrogen to ensure that the magazines remain covered after removal from the robot storage dewar.
6. If a dry shipper is to be used, remove the magazine storage rack from the dry shipper.
7. Remove the storage rack locking bar, used to prevent shifting of the magazines.
8. Use the long tongs to engage the desired magazine at the “ears”. Close the tongs, the locking action will keep them shut. **If the magazine is to be removed from position G, the tongs will have to be rotated 180°**, with the finger holes over the magazine.
9. Place each magazine in the storage rack or into the transfer dewar. Stabilize the storage rack with a gloved hand while sliding the magazine into a slot.
10. Replace the locking bar in the storage rack.
11. Place the foam cover on top of the robot storage dewar.

Appendix A: Magazine location diagram



Appendix B: Error codes and recovery procedures.

Errors may occur during robot operations. Look up the displayed error code in the chart below to determine the appropriate action to take. The errors are organized in groups of 100 numbers, delineated by the robot operation. Robot **normal** status is indicated by a **zero** error number.

	Error	Description	Action to take
Initialization Errors	1	Robot PVs didn't open correctly.	Press start again. This can be repeated up to 3 times if the error reoccurs.
	2	The robot controller failed to start.	Press start again. This can be repeated up to 3 times if the error reoccurs.
	5	An unexpected sample was found.	Enter the hutch and remove the sample, then restart the robot.
	6	A mounted tool was expected.	This is noncritical. A robot mounted phosphor may have be removed by hand.
	7	A mounted sample was expected.	This is noncritical. A robot mounted sample may have be removed by hand.
	10	The beamline was moving during initialization.	Make sure the beamline motors are not moving, then restart the robot.
	11	The robot crashed during initialization.	Check to see if the robot path is clear, then restart the robot.
	12	The E-STOP was pressed.	Restart the robot if ESTOP situation has been cleared.
	13	The light curtain is blocked.	Remove any item from the light curtain beam path, then restart the robot.
	14	The hutch door was open(ed).	Close the hutch door and restart the robot.
Polling	111	There was a crash while the robot was idle.	Remove items from the robot path if necessary, then restart the robot.
	112	The E-STOP was pressed.	Restart the robot if ESTOP situation has been cleared.
	113	The light curtain is blocked.	Remove any item from the light curtain beam path, then restart the robot.
	114	The hutch door was open(ed).	Close the hutch door and restart the robot.
Mounting	201	The beamline was out of position.	Restart the robot and retry operation. If persists, home XY head the try again.
	205	An unexpected sample was found.	Enter the hutch and remove the sample, then restart the robot.
	210	The beamline moved during mounting.	Don't move any equipment while the robot is working, Restart the robot.
	211	The robot crashed during mounting.	Check to see if the robot path is clear, then restart the robot.
	212	The E-STOP was pressed.	Restart the robot if ESTOP situation has been cleared.
	213	The light curtain is blocked.	Remove any item from the light curtain beam path, then restart the robot.
	214	The hutch door was open(ed).	Close the hutch door and restart the robot.
Exchange	301	The beamline was out of position.	Restart the robot and retry operation. If persists, home XY head the try again.
	305	The first sample was not removed	Manualy remove the sample then restart the robot. If error reoccurs contact staff.
	307	A mounted sample was expected.	This is noncritical. A robot mounted sample may have be removed by hand.
	310	The beamline moved during exchange operation.	Don't move any equipment while the robot is working, Restart the robot.
	311	The robot crashed during exchanging.	Check to see if the robot path is clear, then restart the robot.
	312	The E-STOP was pressed.	Restart the robot if ESTOP situation has been cleared.
	313	The light curtain is blocked.	Remove any item from the light curtain beam path, then restart the robot.
	314	The hutch door was open(ed).	Close the hutch door and restart the robot.
Dismount	401	The beamline was out of position.	Restart the robot and retry operation. If persists, home XY head the try again.
	406	A mounted tool was expected.	This is noncritical. A robot mounted phosphor may have be removed by hand.
	407	A mounted sample was expected.	This is noncritical. A robot mounted sample may have be removed by hand.
	410	The beamline moved during dismounting.	Don't move any equipment while the robot is working, Restart the robot.
	411	The robot crashed during exchanging.	Check to see if the robot path is clear, then restart the robot.
	412	The E-STOP was pressed.	Restart the robot if ESTOP situation has been cleared.
	413	The light curtain is blocked.	Remove any item from the light curtain beam path, then restart the robot.
	414	The hutch door was open(ed).	Close the hutch door and restart the robot.
Toolmount	501	The beamline was out of position.	Restart the robot and retry operation. If persists, home XY head the try again.
	505	An unexpected sample was found.	Enter the hutch and remove the sample, then restart the robot.
	510	The beamline moved during tool mounting.	Don't move any equipment while the robot is working, Restart the robot.
	511	The robot crashed during toolmounting.	Check to see if the robot path is clear, then restart the robot.
	512	The E-STOP was pressed.	Restart the robot if ESTOP situation has been cleared.
	513	The light curtain is blocked.	Remove any item from the light curtain beam path, then restart the robot.
	514	The hutch door was open(ed).	Close the hutch door and restart the robot.
Shutdown	611	The robot crashed during toolmounting.	Check to see if the robot path is clear, then restart the robot.
	612	The E-STOP was pressed.	Restart the robot if ESTOP situation has been cleared.
	613	The light curtain is blocked.	Remove any item from the light curtain beam path, then restart the robot.
	614	The hutch door was open(ed).	Close the hutch door and restart the robot.
	620	The operation timed out	Restart the robot and shutdown again.
Park	705	An unexpected sample was found.	Enter the hutch and remove the sample, then restart the robot.
	706	A mounted tool was expected.	This is noncritical. A robot mounted phosphor may have be removed by hand.
	707	A mounted sample was expected.	This is noncritical. A robot mounted sample may have be removed by hand.
	710	The beamline was moving during initialization.	Make sure the beamline motors are not moving, then restart the robot.
	711	The robot crashed during initialization.	Check to see if the robot path is clear, then restart the robot.
	712	The E-STOP was pressed.	Restart the robot if ESTOP situation has been cleared.
	713	The light curtain is blocked.	Remove any item from the light curtain beam path, then restart the robot.
	714	The hutch door was open(ed).	Close the hutch door and restart the robot.